Addendum: ''Bethe stopping-power theory for heavy-target atoms''

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(Received 26 March 1999)

Our previous result on the correction of the Bethe stopping power theory for heavy target elements is amended, with the application of a more consistent version of the semirelativistic Bethe sum rule worked out recently [Phys. Rev. A **57**, 4994 (1998)]. This correction is found to be significant for high-Z target atoms and relatively high-energy incident particles. [S1050-2947(99)01409-2]

PACS number(s): 32.70.Cs, 34.90.+q

In spite of its applicability to relativistic incident particles, it is well known that the Bethe stopping power theory is limited to nonrelativistic target elements with eigenstates satisfying the Schrödinger equation for many-electron atoms. This limitation arises mainly from the derivation of the original Bethe theory, which has applied the various nonrelativistic sum rules (the Bethe and TRK sum rules) [1]. For heavy elements, one would expect a nontrivial correction to the Bethe theory due to the fast motion of the inner shell electrons. This problem was first pointed out by Fano in 1964 in a review of the outstanding unsolved problems in stopping power theory which existed at that time [2]. Since then, to the knowledge of the author, not much effort has been devoted to the study of this problem until recently [3–5]. As also pointed out by Fano in the same review [2], the difficulty in solving this problem lies right in the possible generalization of the various sum rules to the relativistic domain.

Indeed, the relativistic generalization of various atomic sum rules has been an intriguing problem over the past 40 years since the first work on the generalization of the TRK sum rule [6]. It has been studied extensively in the literature using both the single-particle and many-particle (field-theoretic) approaches [7–11]. In a previous attempt, we have used a semirelativistic single-particle approach to obtain the leading relativistic correction terms to the Bethe sum rule [9] and applied the results to derive corrections to the Bethe stopping power theory for heavy target atoms [3]. Unfortunately, it was pointed out later [10] that in most of these previous works based on the same approach [6,7,9,11], there exists an inconsistency in that the transformation of the operator was not included in the Foldy-Wouthuysen transformation performed, which leads to the semirelativistic correction terms for the sum rules. Very recently [12], this error has been corrected and it was found that while the previous corrections to the TRK sum rule were not affected by this error, those for the Bethe sum rule have to be modified.

It is the purpose of this paper to apply these latest corrected results for the semirelativistic sum rules to amend our previous work published in the correction to the Bethe stopping power theory [3]. As before, we shall limit ourselves to the single-particle case and apply the results to a real atom by adopting the independent-particle, local-potential description. Though this seems to be an oversimplified picture, it does have some success in the literature in the analysis of x-ray scattering data using the TRK sum rule [13]. In any case, our preliminary attempt will at least give a first estimate to this effect (due to the relativistic nature of the atomic electrons) as Fano [2] and Bichsel [4] had urged people to study in the previous literature.

We begin by limiting ourselves to the case with nonrelativistic incident particles. In this case, the stopping power obtained from the Bethe theory leads to [1]

$$-\left(\frac{dE}{dx}\right)=\frac{2\pi z^2e^4}{mv^2}N\sum_n\int_{Q_{\min}}^{Q_{\max}}\frac{dQ}{Q^2}\times\left|\left\langle n\left|\sum_{i=1}^{Z}e^{i\vec{q}\cdot\vec{r}_i}\right|0\right\rangle\right|^2(E_n-E_0)=\frac{4\pi z^2e^4}{mv^2}NZ\ell n\left(\frac{2mv^2}{I}\right), \tag{1}$$

where ze and Ze are, respectively, the charge of the incident particle and the target atom, v the velocity of the incident particle, m the mass of the electron, N the number density, and I the mean excitation energy of the target atom. The integration limits for Q ($\equiv\hbar^2q^2/2m$) are given by $Q_{\max}=2mv^2$ and $Q_{\min}=I^2/2mv^2$, respectively [14]. In deriving Eq. (1), we have employed the Bethe sum rule over target atomic states in the form [1]

$$S_1(\vec{q})=\sum_n\left|\left\langle n\left|\sum_{i=1}^{Z}e^{i\vec{q}\cdot\vec{r}_i}\right|0\right\rangle\right|^2(E_n-E_0)=Z\frac{\hbar^2q^2}{2m}\equiv ZQ. \tag{2}$$

Although the Bethe sum in Eq. (2) is often defined with the factor ($\hbar^2q^2/2m$) moved to the left so as to obtain a sum of generalized oscillator strength to depend only on the total charge of the atom, we retain the form as in the above for more convenient application to our present calculation of stopping power to include the correction terms (see below). Note that Eq. (2) is correct only for nonrelativistic target atoms, since $|n\rangle$ in the summation are taken to be eigenstates of the Schrödinger equation for the atoms, and completeness has been applied in its derivation. The generalization of Eq. (2) to account for the relativistic nature of the atomic electrons is nontrivial as already first pointed out by Fano [2].

In our previous works [3,9], we have adopted a semirelativistic single-particle approach to obtain leading-order corrections to Eq. (2), and hence to Eq. (1), by applying the Foldy-Wouthuysen (FW) transformation to the Dirac Hamil-

TABLE I. Comparison of the corrections to the Bethe theory at $K_p = 2$ MeV.

Target Element (Z)	I (eV)[a]	$\lvert E_{tot}\rvert$ (MeV)[b]	Δ_R	C/Z[c]	zL_1[c]	zL_2[c]
Al (13)	164	6.6×10^{-3}	9.7×10^{-3}	2.3×10^{-1}	1.1×10^{-1}	2.2×10^{-2}
Cu (29)	317	4.5×10^{-2}	1.8×10^{-2}	2.8×10^{-1}	8.8×10^{-2}	1.7×10^{-2}
Ag (47)	469	1.5×10^{-1}	2.7×10^{-2}	2.9×10^{-1}	1.1×10^{-1}	2.1×10^{-2}
Au (79)	770	5.2×10^{-1}	4.1×10^{-2}	2.2×10^{-1}	9.8×10^{-2}	1.8×10^{-2}

[a]Reference [16].
[b]Reference [17].
[c]Reference [15].

tonian. It was later pointed out by Aucar, Oddershede, and Sabin [10] that in most of these previous FW approaches to deriving relativistic sum rules [6,7,9,11], there lies an inconsistency in that only the Hamiltonian but not the ''multipole operator'' (i.e., $e^{i\vec{q}\cdot\vec{r}}$ in our case) was subjected to the FW transformation.

Recently [12], we have fixed this inconsistency and have obtained a more correct version for the semirelativistic corrections to Eq. (2). For a one-particle system with the ground state being described by a spherical symmetric hydrogenic wave function, the Bethe sum rule to $O(v^2/c^2)$ of the atomic electron can be obtained as

$$S_1(\vec{q}) = \frac{\hbar^2 q^2}{2m} - \frac{5\hbar^4 q^2 Z^2}{12 m^3 c^2 a^2} - \frac{\hbar^4 q^4}{4 m^3 c^2}, \tag{3}$$

where a is the Bohr radius. The only correction from this more consistent treatment in this case occurs in the q^4 term, which is twice as large compared to the previous result [3,9] where the operator $e^{i\vec{q}\cdot\vec{r}}$ was not transformed. To apply this result to the case of a many-electron atom, we follow the independent-particle, local-potential approach of Smith [13], which has been found to be reasonable in the analysis of anomalous x-ray scattering data. Adopting this picture and with the application of the virial theorem [3,13], we then obtain a corrected form of Eq. (2) to $O(v^2/c^2)$ of the atomic electrons in the form

$$\begin{aligned} S_1(\vec{q}) &= \sum_n \left| \left\langle n \left| \sum_{i=1}^{Z} e^{i\vec{q}\cdot\vec{r}_i} \right| 0 \right\rangle \right|^2 (E_n - E_0) \\ &= Z \frac{\hbar^2 q^2}{2m} \left[1 - \frac{5}{3} \frac{|E_{\text{tot}}|}{Zmc^2} - \frac{1}{2} \left(\frac{\hbar q}{mc} \right)^2 \right], \end{aligned} \tag{4}$$

where $E_{\text{tot}}(<0)$ is the ground-state binding energy of the atom. Applying this result to the calculation of stopping power in Eq. (1), we finally obtain the semirelativistic correction terms for heavy target elements to the Bethe nonrelativistic formula as follows:

$$\begin{aligned} -\left(\frac{dE}{dx}\right) &= \frac{4\pi z^2 e^4}{mv^2} NZ \ell n \left(\frac{2mv^2}{I} \right) \\ &\times \left[1 - \frac{5}{3} \frac{|E_{\text{tot}}|}{Zmc^2} - \frac{1}{\ell n\left(\frac{2mv^2}{I}\right)} \frac{(Q_{\max} - Q_{\min})}{2mc^2} \right], \end{aligned} \tag{5}$$

which leads to a correction of a factor 2 for the last term compared with previous result [3], where the more consistent sum rule Eq. (4) was not applied. To put these correction terms in the right perspective, let us rewrite the Bethe formula to incorporate several other well-known corrections together with those as revealed in Eq. (5) in the following form [15,16]:

$$\begin{aligned} -\left(\frac{dE}{dx}\right) = \frac{4\pi z^2 e^4}{mv^2} NZ \bigg[\ell n \left(\frac{2mv^2}{I} \right) \\ - C/Z + zL_1 + z^2 L_2 - \Delta_R \bigg], \end{aligned} \tag{6}$$

where $-C/Z$ is the shell correction, zL_1 the Barkas effect, and $z^2 L_2$ the Bloch correction, respectively. Δ_R is the present correction term given by

$$\Delta_R = \tfrac{5}{3} \ell n \left(\frac{2mv^2}{I} \right) \frac{|E_{\text{tot}}|}{Zmc^2} + \frac{(Q_{\max} - Q_{\min})}{2mc^2}. \tag{7}$$

Note that although the previous result did not derive the last term in Eq. (7) correctly, it was nevertheless neglected in the previous numerical computation [3]. Here we illustrate the effect of this corrected formula Eq. (7) with both terms included. New numerical results (together with a comparison with other corrections) are obtained as shown in Tables I and II, where we have assumed the incident particle to be a proton with energy equal to K_p. From these results one can draw the following conclusions: (i) the present correction is important for large-Z target elements and can become comparable to the Barkas and Bloch terms for these elements; and (ii) for the same target element, the present correction

TABLE II. Δ_R as a function of incident proton energy.

K_p / Δ_R / Z	2 MeV	10 MeV	50 MeV
Al (13)	9.7×10^{-3}	2.9×10^{-2}	1.2×10^{-1}
Cu (29)	1.8×10^{-2}	4.3×10^{-2}	1.4×10^{-1}
Ag (47)	2.7×10^{-2}	6.1×10^{-2}	1.6×10^{-1}
Au (79)	4.1×10^{-2}	9.3×10^{-2}	2.1×10^{-1}

becomes more significant for incident particles of higher energy. To access more accurately the effect observed in (ii), one has to generalize the present treatment to the case of a relativistic incident particle—thus anticipating corrections to the relativistic Bethe formula [1]. This turns out to be a very challenging problem and we hope future endeavors will help to settle this issue.

We thank S. M. Cohen for a useful contribution to the sum-rule work, and the Faculty Development Grant of Portland State University for partial support of this work.

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